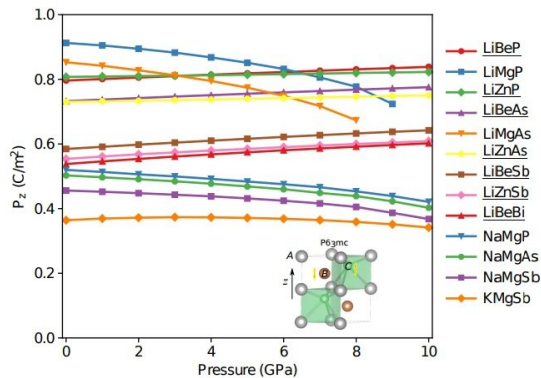


Negative piezoelectric effect is not so rare after all

30 November 2017, by Lisa Zyga



A comparison of ferroelectric materials, some of which exhibit the negative longitudinal piezoelectric effect. Materials with pressure-enhanced ferroelectricity are underlined. Credit: Liu et al. ©2017 American Physical Society

(Phys.org)—The piezoelectric effect, which causes a material to expand along the direction of an applied electric field, is common in many materials and used in a variety of technologies, from medical ultrasound to vibration-powered electronics. But the negative piezoelectric effect, in which a material contracts rather than expands in the direction of the applied electric field, has been considered a rare and counterintuitive anomaly, and has received little attention.

Now in a new paper published in *Physical Review Letters*, physicists Shi Liu and R. E. Cohen at the Carnegie Institute for Science in Washington, D.C., have identified 93 materials that exhibit the negative piezoelectric effect, showing that it is much more common than previously thought. They also investigated the origins of the negative piezoelectric effect, which may lead to the development of new piezoelectric devices.

"The negative longitudinal piezoelectric effect was

not well-examined in the past," Cohen told *Phys.org*. "Our paper is the first work to carry out a systematic investigation of the mechanism of the negative piezoelectric effect. Taking advantage of the well-curated open-source materials database hosted by the Materials Project, we are able to quickly identify nearly 100 materials possessing this unusual response literally within minutes. This work highlights how detailed quantum mechanical calculations and material informatics can work together to accelerate materials discovery and design."

As the researchers explained, piezoelectricity contains two components: a clamped-ion contribution, which is purely electronic, and an internal-strain contribution, which arises from microscopic atomic relaxations.

In the new study, the physicists discovered that the key difference between conventional and negative piezoelectric materials is which contribution is larger. In conventional piezoelectrics, the internal-strain contribution dominates, while in negative piezoelectrics the clamped-ion response dominates, indicating the presence of strong ionic bonds and small atomic relaxations in these materials.

The researchers then searched an existing database of nearly 1000 piezoelectric materials and identified 93 compounds possessing a dominant clamped-ion component, marking them as negative piezoelectrics.

In their analysis, the physicists also discovered another unusual characteristic of negative piezoelectric materials, which is that high pressure enhances their ferroelectricity. This is the opposite of what is observed in conventional piezoelectric materials, where high pressures cause a decrease in ferroelectricity. The researchers hope that this pressure-enhanced ferroelectricity of negative piezoelectric materials may lead to the design of

new devices.

"This work illustrates the power of theory and informatics together, and we (and others) can use this approach to find other new kinds of interesting [materials](#)," Liu said. "Regarding piezoelectrics, we hope this work will inspire experimental studies of the negative longitudinal piezoelectric effect. Our colleagues here are working to synthesize some of the compounds with negative [piezoelectric](#) response we proposed in the paper. It will also be very interesting to investigate what will happen if we create a composite material system with alternating layers of conventional piezoelectrics with positive response and those with negative response. When you turn on the [electric field](#), some layers will expand whereas some layers will contract. Such competition may give rise to unusual physics and potentially enable new applications."

More information: Shi Liu and R. E. Cohen.

"Origin of Negative Longitudinal Piezoelectric Effect." *Physical Review Letters*. DOI:

[10.1103/PhysRevLett.119.207601](https://doi.org/10.1103/PhysRevLett.119.207601)

Also at [arXiv:1708.07240](https://arxiv.org/abs/1708.07240) [cond-mat.mtrl-sci]

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